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Neurocomputing helps design new materials

by Fred Coleman, Materials and Manufacturing Directorate

WRIGHT-PATTERSON AFB, OHIO — How many different useful materials are there? If one were to consider the possible number of just two, three or four element combinations of the roughly 100 elements, the number of compounds and solutions that would result is in the billions.

Scientists in the Air Force Research Laboratory Materials and Manufacturing Directorate, interested in seeking a computational approach to predicting the existence of a multi-element compound, sponsored a collaborative research effort that led to a significant breakthrough in using neural networks to help design new materials.

The team discovered that a nonlinear expression involving an elementary material property could be used to predict, with greater than 99 percent accuracy, the existence of a compound for a multi-element materials system. This discovery will result in significant savings of time and resources and will speed the search for future, yet-to-be realized materials.

There are about 5,000 binary (composed of two elements), 162,000 ternary (three element), and roughly four million quaternary (four element) materials systems possible," according to Dr. Steven R. LeClair, Materials scientist and chief of the directorate's Process Design Branch.

"Of course, many of these combinations do not form compounds, and of those that do, data exists for only 80 percent of the binary systems, five percent of the ternary systems, and less than one percent of the quaternary systems," LeClair said.

LeClair's branch, together with the Air Force Office of Scientific Research, provided funding to Dr. Pierre Villars, of Switzerland, to establish an international research project, which addressed strategies for accelerating materials design. Villars is a world-renowned expert in crystallography and a source for many of the world's materials data handbooks. The project took advantage of Villars' access to quality materials data and leveraged an existing AFOSR initiative referred to as Electronic Prototyping, involving basic research in recursive linear regression and adaptive stochastic optimization as applied to function approximation.

"Electronic Prototyping is a research effort wherein the goal is for all devised artifacts to be prototyped electronically to simulate shape, processing and operation in an intended environment," LeClair explained. "The objectives of this initiative are to develop new computational methods to model and relate materials-product-process designs; to integrate, synthesize and generalize new knowledge; and to automate knowledge discovery for use in improving productivity."

By combining their expertise, and leveraging resources, in April 1999, Villars and the Electronic Prototyping research team made a significant breakthrough. They discovered that a nonlinear expression involving an elemental property could be used to predict the occurrence of a compound for a multi-element (binary, ternary, etc.) materials system. The material property, referred to as the Mendeleev Number, was originally conceived by D.G. Pettifor, of Oxford University, England, to group binary compounds by structure type.

"This discovery will save a tremendous amount of time and resources in the exploration of future, yet-to-be-realized, materials systems, particularly the four million quaternary systems on which there is little data," LeClair said. "These quaternary systems include high temperature superconductors, photonics/optical semiconductor, piezoelectrics and a host of other compounds exhibiting unique combinations of properties which will enable new, more advanced technologies for tomorrow's Air Force. We now have a computational approach to determining which combinations of elements will yield compounds that may lead to potentially useful materials.

The long term goal of the projects to discover continued research of methods to predict specific combinations of properties, which ultimately will enable an end-user to select a material or material alternatives by simply specifying operational requirements, LeClair said.

In addition to Villars and LeClair, the team members included: Professor Bhavik Bakshi, Ohio State University; Professor Phillip Chen, Wright State University; Dr. Boris Igelnik, Case Western University; Dr. Al Jackson, Technical Management Concepts, Incorporated; Professor Mike Kirby, Colorado State University; Professor Mark Oxley, Air Force Institute of Technology; and Professor Yoh-Han Pao, Case Western University. **@**